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## **2.1 Å Crystal Structure of 53-mer Domain I RNA.**

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The crystal structure of the 53-mer RNA from *T. aquaticus*, which corresponds to nucleotides 299-253 in *H. marismortui*, has been determined at 2.1 Å resolution. The crystals belong to the P43212 space group with unit cell dimensions  $a=b=42.37$  Å,  $c=151.51$  Å. The structure was solved by molecular replacement using AmoRe program and refined with Refmac program. The final model contains one 53-mer RNA molecule, two Mg<sup>2+</sup> ions, five Ca<sup>2+</sup> ions, eight Os<sup>4+</sup> ions and 157 water molecules with R-factor = 17.9% (R-free=23.3%) using all data with  $F > 0$ .

The free 53-mer RNA in the presence of cations adopts the native structure, including all tertiary contacts identified previously in the mature 50S ribosome [1]. The 2.1 Å structure of the 53-mer RNA identified two pairing alignments involving syn bases that are crucial for maintaining a loop-loop self-kissing structure.

We also obtained crystals of the mutant RNA (G308U) at 3 Å resolution. The crystals belong to the P43212 space group with unit cell dimensions  $a=b=46.8$  Å,  $c=160.0$  Å. The final model contains one 53-mer RNA molecule, four Mg<sup>2+</sup> ions with R-factor = 24.8% (R-free=27.3%) using all data with  $F > 0$ . The G308U mutation of the 53-mer RNA creates a A-U pair instead of a non-canonical G-A pair. This replacement changes the shape of the surface for L24 recognition.

1. D.J. Klein, T.M. Schmeing, P.B. Moore, T.A. Steitz  
The Kink-Turn: A New RNA Secondary Structure Motif  
EMBO J., 20, pp. 4214-4221, 2001.

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